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AUTOIGNITION AND COMBUSTION OF DIESEL AND JP-8

(Grant/Contract Number 45241-EG)

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SUMMARY/OVERVIEW:

Experimental and numerical studies are carried out to construct reliable surrogates that can reproduce aspects of combustion of JP-8 and Jet-A. The combustion characteristics considered are extinction and autoignition in laminar non premixed flows. Three surrogates are constructed. The measured values of the critical conditions of extinction and autoignition for the surrogates are compared with those for the jet fuels. Numerical calculations are carried out using a semi-detailed chemical-kinetic mechanism. The calculated values of the critical conditions of extinction and autoignition for the surrogates are found to agree well with experimental data. The research is performed in collaboration with Professor Eliseo Ranzi at Politecnico di Milano, Italy.

TECHNICAL DISCUSSION:

The major components of jet fuels are straight chain paraffins, branched chain paraffins, cycloparaffins, aromatics, and alkenes [1, 2]. Surrogate fuels are defined as mixtures of few hydrocarbon compounds whose relative concentrations can be adjusted so that the physical and chemical properties pertinent to combustion approximate those for jet fuels. Starting from the pioneering work of Schulz [3], who proposed a 12-component surrogate mixture for JP-8, several investigators have proposed surrogates for jet fuels. Examples are the Drexel surrogate of Ref. [4] and the Utah surrogate of Ref. [5]. Here three surrogates labeled (A), (B), and (C) are constructed and tested. The composition of these surrogates are

Surrogate (A) : 60 % *n*-decane, 20 % methylcyclohexane, and 20 % toluene.

Surrogate (B) : 60 % *n*-decane, 20 % methylcyclohexane, and 20 % *o*-xylene.

Surrogate (C) : 60 % *n*-dodecane, 20 % methylcyclohexane, and 20 % *o*-xylene.

Experiments are carried out employing the counterflow configuration. The burner used in the experimental study is made up of two ducts. A fuel stream made up of prevaporized fuel and nitrogen is injected from the fuel-duct, and an oxidizer stream of air is injected from the oxidizer-duct. Critical conditions of extinction are presumed to be given by the strain rate, $a_{2,e}$, and the mass fraction of fuel, $Y_{F,1}$, at the fuel boundary. Critical conditions of autoignition are presumed to be given by the strain rate, $a_{2,I}$, the temperature of the oxidizer

stream, $T_{2,I}$, and the mass fraction of fuel, $Y_{F,1}$, at the fuel boundary. The strain rate is calculated using the injection velocities of the counterflowing streams at the boundaries [6].

Experiments are carried out at a pressure of 1.013 bar. In the extinction experiments the temperature of the fuel stream is $T_1 = 503 (\pm 10)$ K, and the temperature of the oxidizer stream, $T_2 = 298$ K. The accuracy of the strain rate is $\pm 10\%$ of recorded value and that of the fuel mass fraction $\pm 3\%$ of recorded value. The experimental repeatability on reported strain rate is $\pm 5\%$ of recorded value. In the autoignition experiments the temperature of prevaporized fuel and nitrogen at the fuel boundary was maintained at 503 K. The temperature of air was increased until autoignition takes place. The accuracy of the measurement of the temperature of air at autoignition is expected to be ± 30 K, the strain rate $\pm 10\%$, and fuel mass fraction $\pm 3\%$ of recorded value. The experimental repeatability in the measurement of the temperature of air at autoignition is expected to be ± 6 K.

Numerical calculations were performed by Professor Eliseo Ranzi at Politecnico di Milano, Italy, using the chemical-kinetic in Ref. [7]. The high molecular weight compounds, used as reference fuels here, undergo a sequential reduction to lower molecular weight hydrocarbons during combustion. The semi-detailed approach uses a lumped description of the primary propagation reactions for the large species to smaller species, and then treats the successive reactions of smaller species with a detailed chemical-kinetic scheme. The overall chemical-kinetic scheme for the simulation of pyrolysis and combustion of high molecular weight hydrocarbon fuels, including those for the reference fuels considered here, is made up of 7878 reactions among 283 species. The computational model used here is a modified version of the opposed-flow diffusion flame code (OPPDIF [8]). The boundary conditions employed in the calculations are identical to those in the experiments. Flame structures and critical conditions of extinction and autoignition are obtained.

First, numerically calculated values of the critical conditions of extinction and autoignition of the reference single component fuels are compared with measurements. Next, similar comparisons are made for the surrogates (A), (B), and (C). Selected results are shown in Figs. 1, 2, and 3. The symbols in these figures represent experimental data, and the lines are results of numerical calculations. Figure 1 shows the temperature of the oxidizer stream at autoignition as a function of the strain rate for *n*-decane, *n*-dodecane, methylcyclohexane, and toluene. This figure shows data obtained at a fixed value of the mass fraction of fuel in the fuel stream $Y_{F,1} = 0.3$. The numerical results agree well with experimental data. Figure 2 shows the mass fraction of fuel as a function of the strain rate at extinction. The experimental data for surrogates are compared with those for JP-8 and Jet-A. Figure 2 shows that the extinction characteristics of JP-8 and Jet-A are similar. Moreover the extinction characteristics of the mixture (C) are close to those for JP-8 and Jet-A. Figure 3 shows the temperature of the oxidizer stream at autoignition as a function of the strain rate for the surrogates. Figure 3 shows that the fuel mixtures are slightly more reactive than Jet-A. The autoignition characteristics of mixture (C) are closest to those for Jet-A.

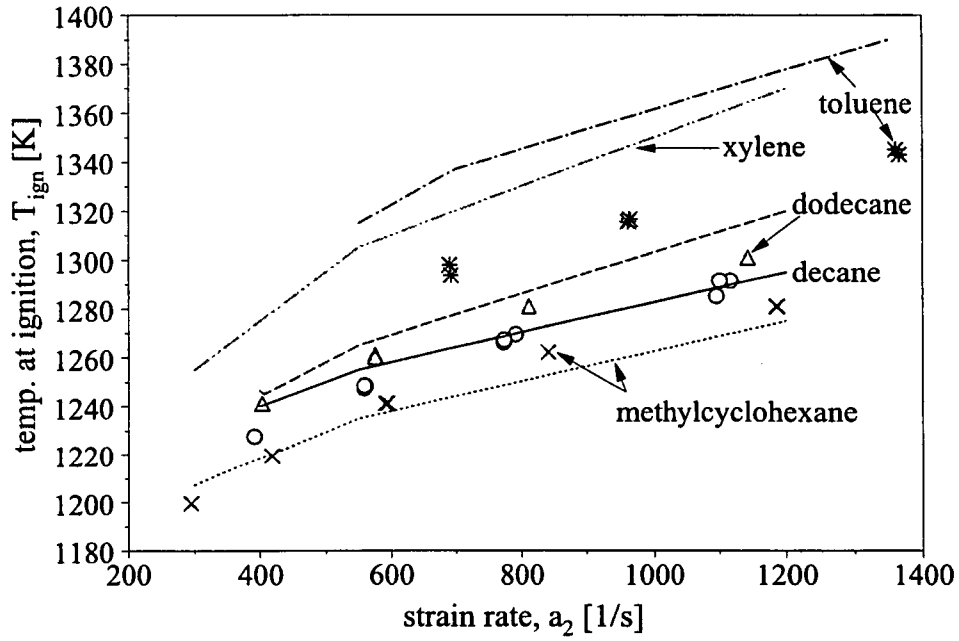


Figure 1: The temperature of the oxidizer stream at autoignition as a function of the strain rate. The figure shows experimental data obtained at fixed values of the mass fraction of fuel in the fuel stream $Y_{F,1} = 0.3$.

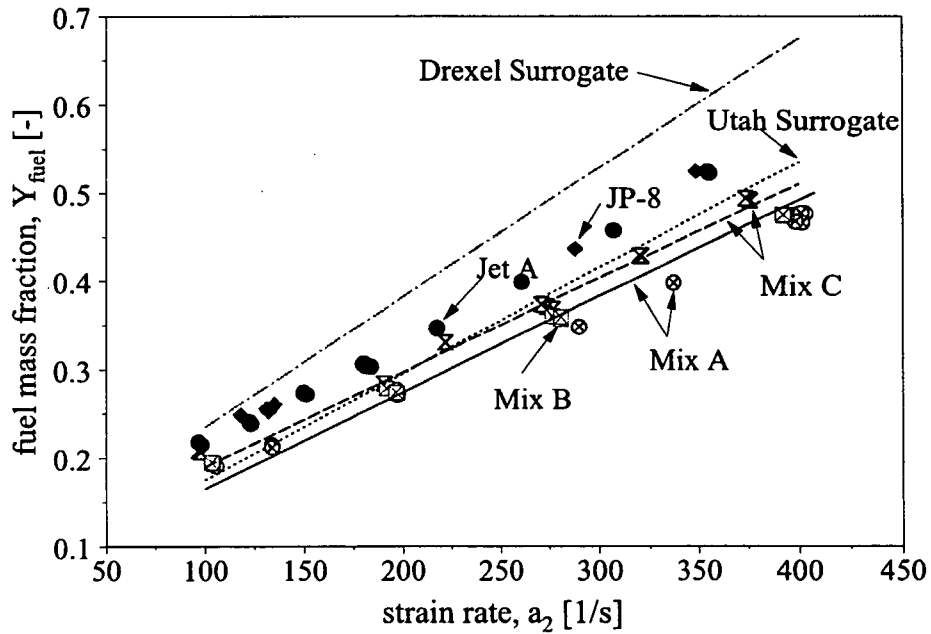


Figure 2: The mass fraction of fuel as a function of the strain rate at extinction.

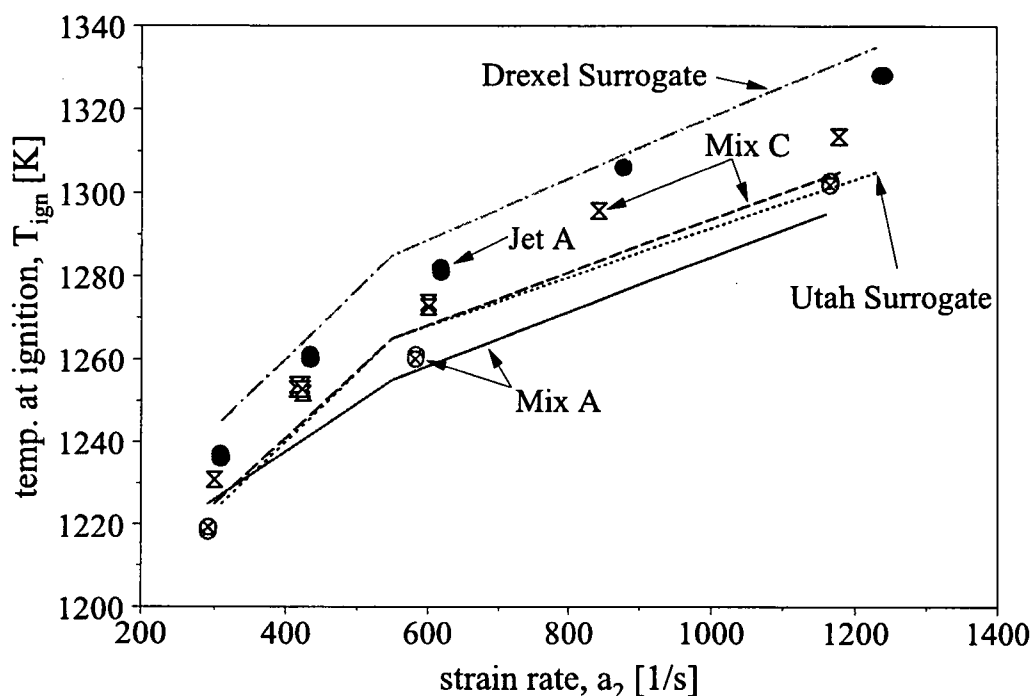


Figure 3: The temperature of the oxidizer stream at autoignition as a function of the strain rate.

References

- [1] T. Edwards, L. Q. Maurice, *Journal of Propulsion and Power* 17 (2001) 461–466.
- [2] T. Edwards, *2001 Fall Technical Meeting, Eastern States Section of the Combustion Institute*.
- [3] W. Schulz, *ACS Petroleum Chemistry Division Preprints* 37 (2) (1991) 383–392.
- [4] A. Agosta, N. P. Cernansky, D. L. Miller, T. Faravelli, E. Ranzi, *Experimental Thermal and Fluid Science* 28 (2004) 701–708.
- [5] A. Violi, S. Yan, E. G. Eddings, A. F. Sarofim, S. Granata, T. Faravelli, E. Ranzi, *Combustion Science and Technology* 174 (2002) 399–417.
- [6] K. Seshadri, F. A. Williams, *International Journal of Heat and Mass Transfer* 21 (2) (1978) 251–253.
- [7] <http://www.chem.polimi.it/CRECKModeling>.
- [8] A. Lutz, R. Kee, J. Grcar, F. Rupley, Tech. Rep. SAND96-8243, Sandia National Laboratories (1997).